Peridynamic Modeling of Material Failure

Stewart Silling

Computational Physics Department
Sandia National Laboratories
Albuquerque, NM 87185-0378
sasilli@sandia.gov

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy under contract DE-AC04-94AL85000.

Supercomputing at Berkeley when I was a student

CDC 6600: 10MHz

Seymour Cray

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Collaborators

- Prof. Rohan Abeyaratne, Markus Zimmermann, and Olaf Weckner (MIT)
- Abe Askari, John Haws, and Xifeng Xu (Boeing)
- Prof. Kaushik Bhattacharya and Kaushik Dayal (Caltech)
- Prof. Florin Bobaru (University of Nebraska)
- Paul Demmie (Sandia)
- Simon Kahan (Cray)
- Prof. Walter Gerstle (University of New Mexico)
- Kirsten Fagnon (University of Washington)

Sponsors

- US Department of Energy
- DoD/DOE Joint Munitions Technology Program
- US Nuclear Regulatory Commission
- The Boeing Company

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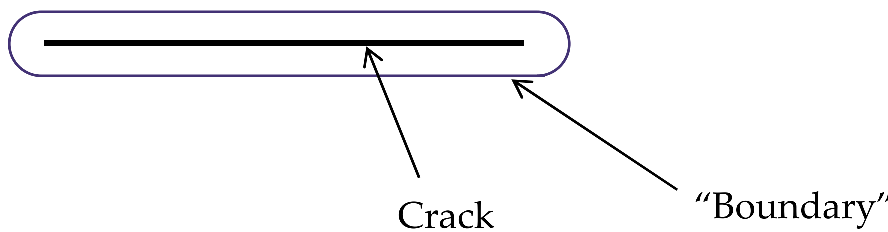
A problem with the classical theory

- PDEs don't apply when a crack or other discontinuity appears.
  - So cracks have to be treated by special techniques.
  - Example: redefine the body to exclude a crack:



(This doesn't work too well if you don't know where the crack is!)

- Purpose of the <u>peridynamic</u> model:
  - <u>Reformulate the basic equations so that they hold everywhere in a body regardless of discontinuities.</u>

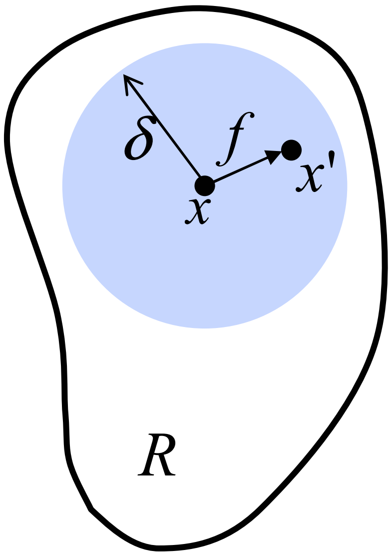
Peridynamic* model

- Replace the $\nabla \cdot \sigma$ term in the equation of motion:

$$\rho \ddot{u}(x,t) = \int_R f(u' - u, x' - x)\, dV' + b(x,t)$$

- Note the similarity to molecular dynamics.
- f is the force that x' exerts on x per unit volume squared, dependent on:
  - relative position in the reference configuration,
  - relative displacement,
  - (will consider history dependence later).
- **Not** obtainable by applying the divergence theorem to the classical PDE.
- Convenient to assume f vanishes outside some <u>horizon</u> d.
- Require:

$$f(-\eta, -\xi) = -f(\eta, \xi) \qquad f(\eta, \xi) \times (\eta + \xi) = 0$$



* From the Greek "near" + "force"

Some references

- Similar idea proposed for multiscale (linear only):
  - I. A. Kunin, *Elastic Media With Microstructure* (1982).
  - D. Rogula, *Nonlocal Theory of Material Media* (1982).

- 3D nonlinear theory:
  - S. A. Silling, Reformulation of elasticity theory for discontinuities and long-range forces, *JMPS* (2000).
  - M. Zimmermann, thesis (to appear).

- Analytical approaches to 1D problems:
  - S.A. Silling, M. Zimmermann, and R. Abeyaratne, Deformation of a peridynamic bar, *Journal of Elasticity* (2003).
  - O. Weckner and R. Abeyaratne, The effect of long-range forces on the dynamics of a bar, *JMPS* (to appear).

- Numerical method:
  - S.A. Silling and E. Askari, A meshfree method based on the peridynamic model of solid mechanics, *Computers and Structures* (to appear).

- Fracture and damage (mostly numerical):
  - S.A. Silling and E. Askari, Peridynamic modeling of impact damage, ASME PVP-Vol. 489 (2004).
  - S.A. Silling and F. Bobaru, Peridynamic modeling of membranes and fibers, *International Journal of Non-Linear Mechanics* (2005).

- Phase boundaries:
  - K. Dayal, thesis (to appear).

Microelastic materials

- A body is <u>microelastic</u> if f is derivable from a scalar **micropotential** w, i.e.,

$$f(\eta,\xi)=\frac{\partial w}{\partial \eta}(\eta,\xi) \qquad \eta = u'-u \qquad \xi = x'-x$$

- Interactions ("bonds") can be thought of as elastic (possibly nonlinear) springs.
- Elastic energy is stored reversibly:

$$\dot{\Phi}=\int_R b\cdot\dot{u}dV$$

  – where the strain energy density is

$$W(x)=\frac{1}{2}\int_R w(u'-u,x'-x)dV'$$

  – and the total strain energy is

$$\Phi=\int_R W(x)dV$$

- Can show (using Stokes' theorem) that the force magnitude depends on $\boldsymbol{\eta}$ only through the current scalar distance between $\boldsymbol{x}$ and $\boldsymbol{x}'$.

$$w(\eta,\xi)=\hat{w}(|\xi+\eta|,\xi)$$

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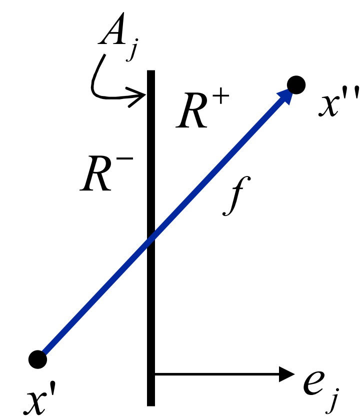
Relation to classical theory

- For a given microelastic material with micropotential *w*, we can *define* a **classical hyperelastic** material through

$$\hat{W}(F) = \frac{1}{2}\int_R w((F-1)x, x'-x)\,dV'$$

- Can *define* a stress-like quantity

$$\sigma_{ij}(x) = \lim_{A_j \to 0}\left\{\frac{1}{A_j}\int_{R^+}\int_{R^-} f_i(u''-u', x''-x')\,dV''dV'\right\}$$

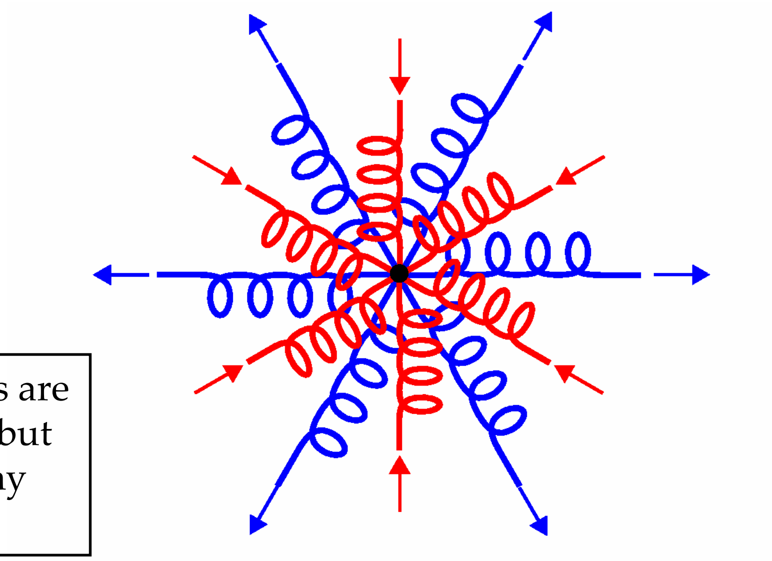


but this is meaningful only for homogeneous deformations.

- Can show that the peridynamic equation of motion "converges to" the classical version in the limit $\delta \to 0$.

Unstressed configurations

- Forces between particles can be nonzero even when the "stress" vanishes.
- Could make this an attractive approach for "multiscale" modeling.



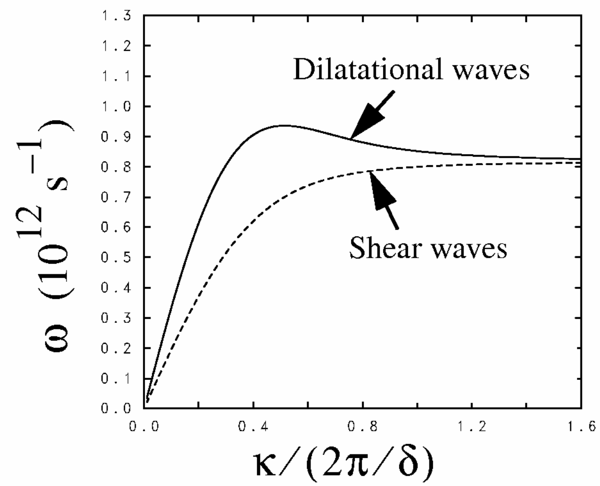
<u>Unstressed</u>: Bond forces are not only equilibrated, but their sum through any surface vanishes.

Relation to classical theory, ctd.

- Can show that an unbounded, homogeneous, isotropic peridynamic body sustains two types of small-amplitude waves:

$$\underset{\sim}{u}(\underset{\sim}{x}, t) = \underset{\sim}{a} e^{i(\kappa \underset{\sim}{N} \bullet \underset{\sim}{x} - \omega t)}.$$

  – Longitudinal (displacement parallel to propagation direction)
  – Shear (displacement orthogonal to propagation direction)
  – But these waves are dispersive.



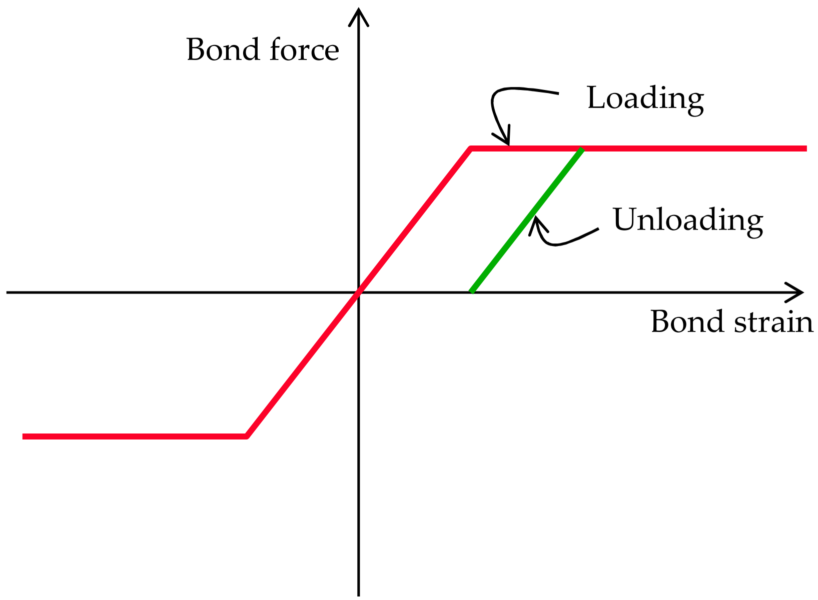
Typical dispersion curves

Other constitutive models

- Visco-microelastic:

$$f(r, \dot{r}, \xi), \qquad r = |\xi + \eta| = \text{current distance between } x \text{ and } x'$$

- Microplastic:



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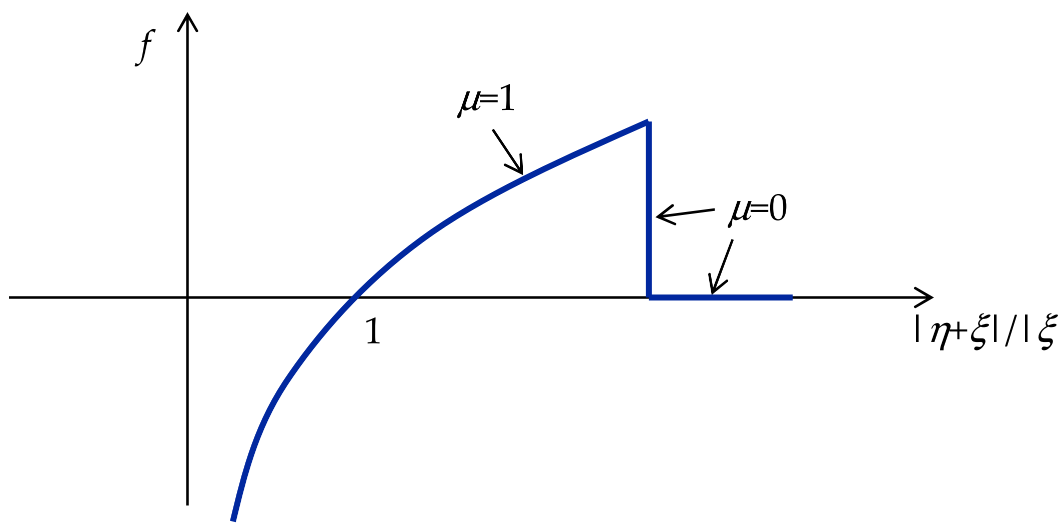
Damage

- Damage is introduced at the bond level:

$$\bar{f}(\eta,\xi,x,t) = f(\eta,\xi)\mu(\xi,x,t)$$

where μ =1 for an intact bond, 0 for a broken bond.

- Bond breakage occurs irreversibly according to some criterion such as exceeding a prescribed critical stretch.



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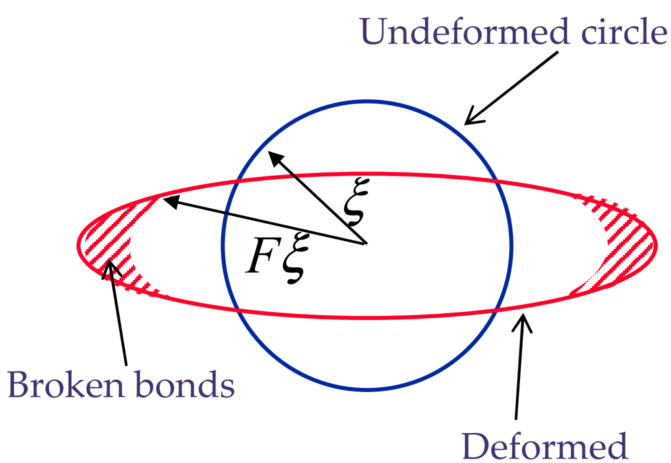
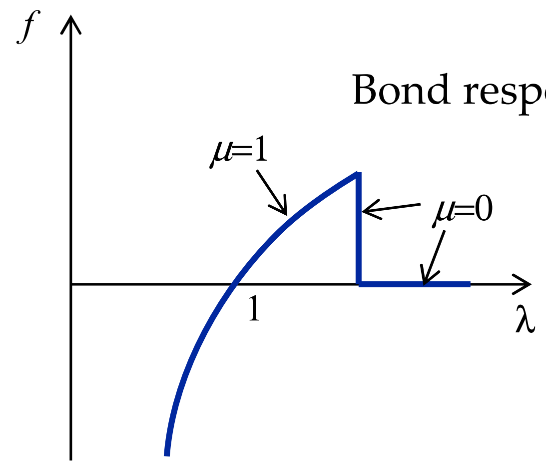
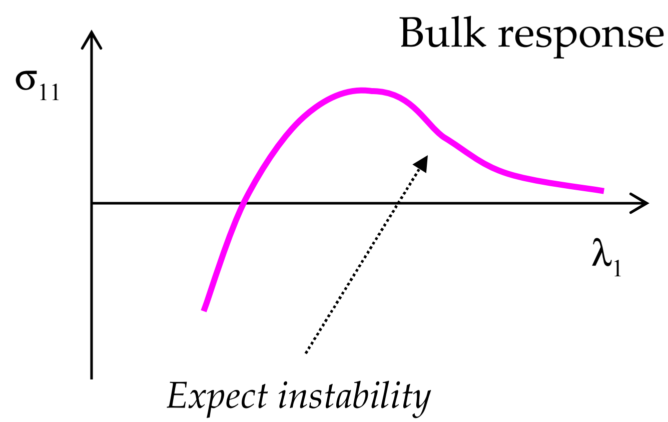
Bulk response with damage

- Assume a homogeneous deformation.







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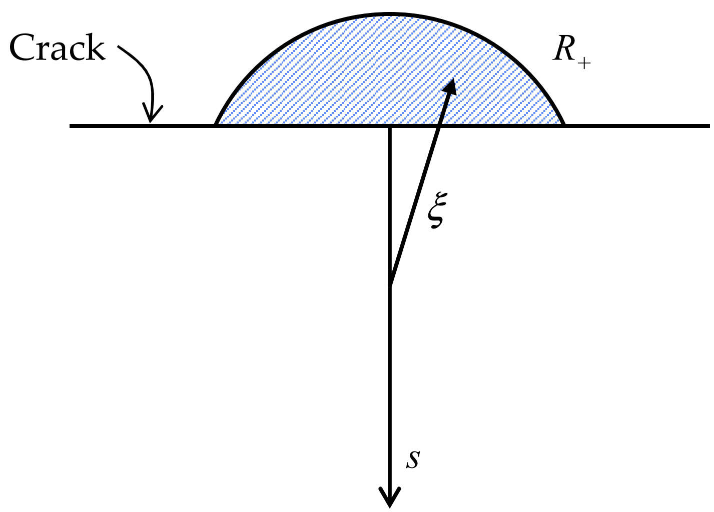
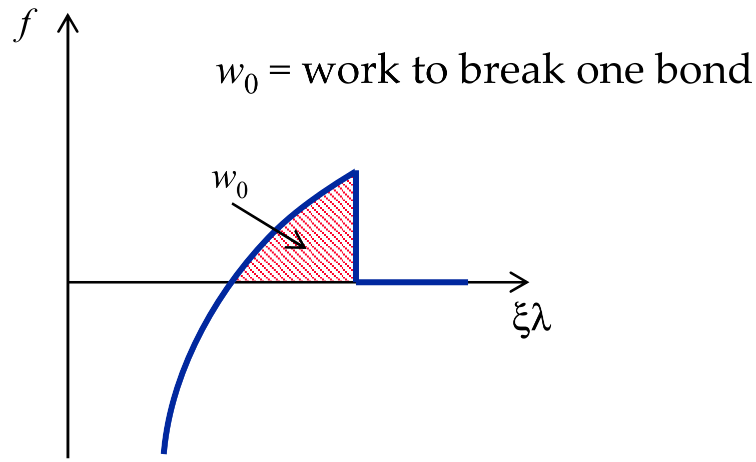
Energy required to advance a crack

- Adding up the work needed to break all bonds across a line yields the energy release rate:

$$G = 2h \int_0^{\delta} \int_{R_+} w_0 \, dV \, ds$$





There is also a version of the J-integral that applies in this theory.

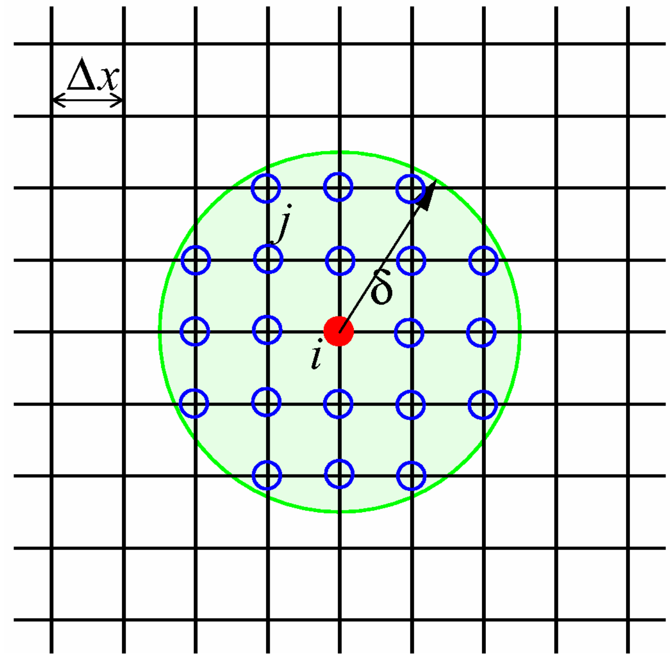
Numerical method

- Replace the integral in the equation of motion by a finite sum:

$$\rho \ddot{u}(x,t) = \int_R f(u'-u, x'-x)\,dV' + b(x,t)$$

is approximated by

$$\frac{\rho}{\Delta t^2}\left(u_i^{n+1} - 2u_i^n + u_i^{n-1}\right) = \sum_{|x_j - x_i| < \delta} f(u_j^n - u_i^n, x_j - x_i)(\Delta x)^3 + b_i^n$$



Special case of a cubic grid

- Method is "meshless Lagrangian".
  - no elements
  - error is $O(\Delta x^2)$ if u is continuous.
- Sandia 3D peridynamic code is called Emu.
  - available under license from Sandia

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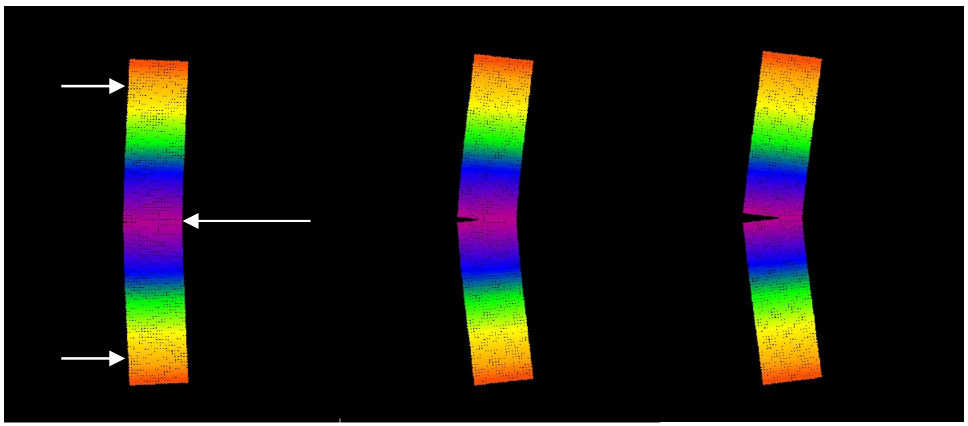
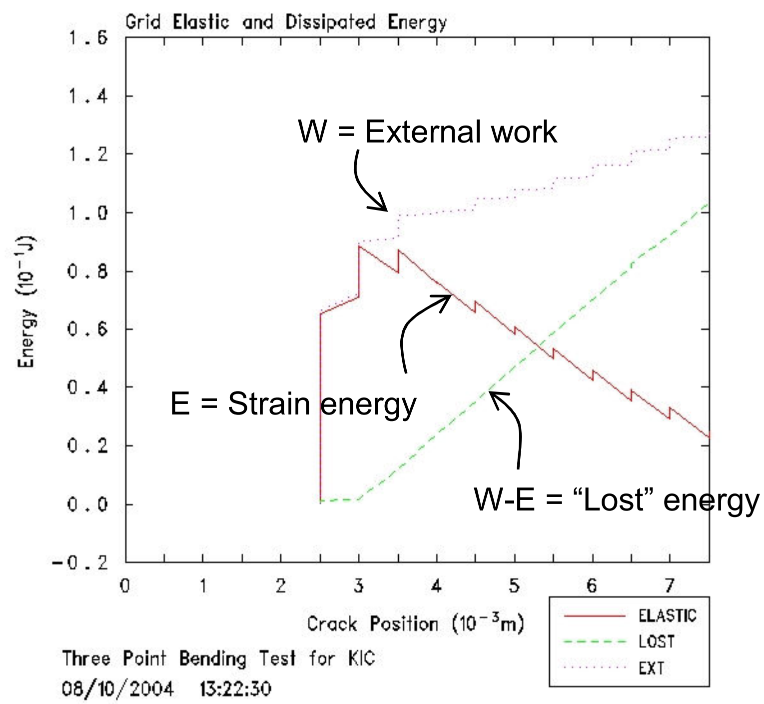
3-point bend test in a metal: Emu model

- 2D model of ASTM standard test for KIc.





Energy as a function of crack length

- Constant slope of the "lost" energy curve is the energy release rate G.
- Confirms that the code accurately models fracture under the assumption of constant KIc.
- Also shows how this quantity depends on model parameters.

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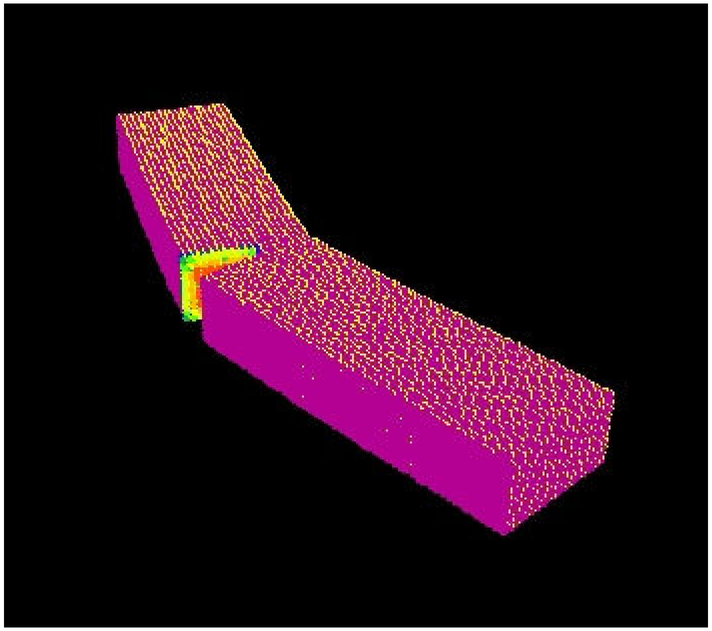
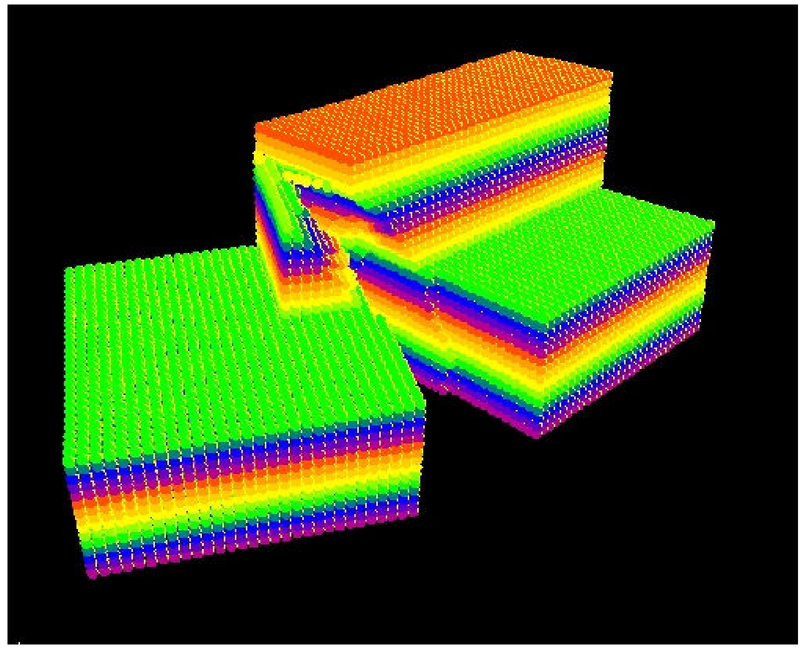
Single crack growth in metals: 3D model

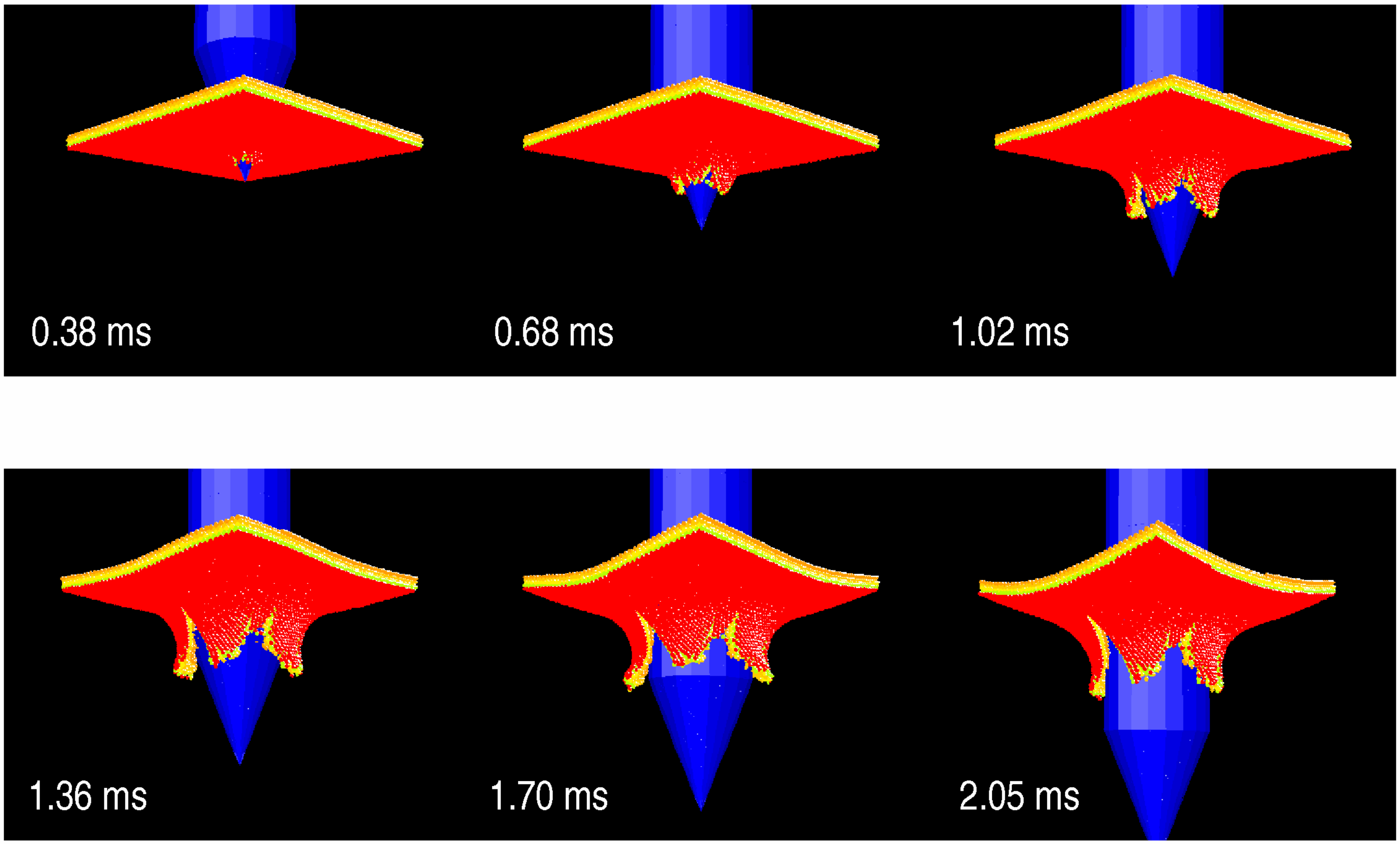


3-point bend



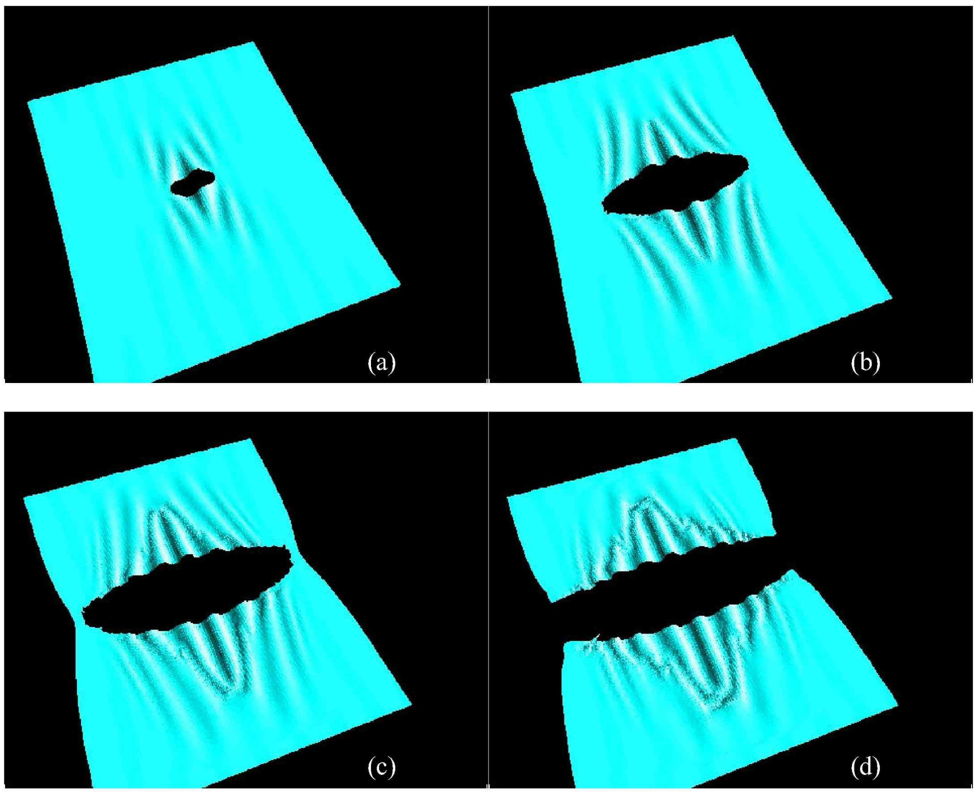
A more complex geometry

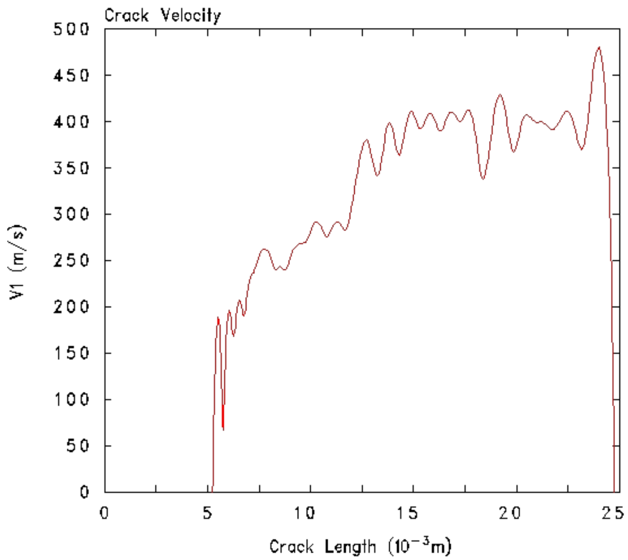
Petaling in perforation of a ductile plate



Dynamic fracture:
Tearing of a membrane

- Wrinkles appear due to compressive strains parallel to the crack*.





Crack tip velocity

*Also see Haseganu and Steigmann, *Computational Mechanics* (1994) for numerical model of wrinkling.

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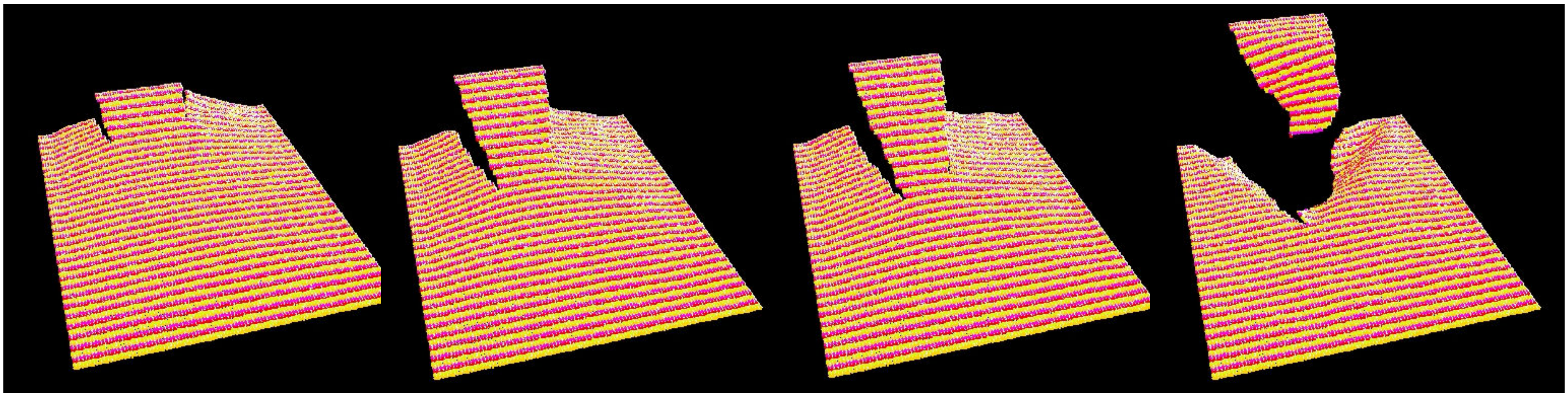
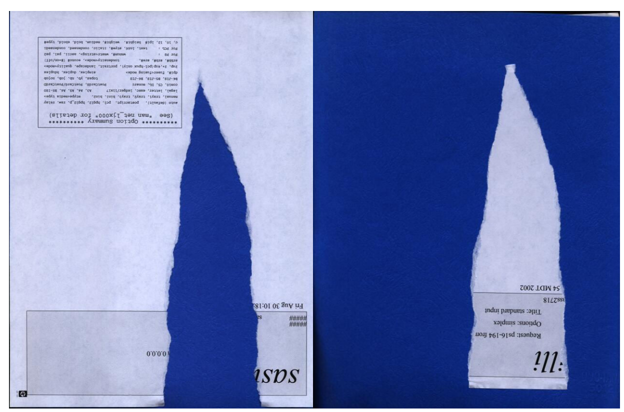
Interaction of 2 cracks:
Peeling of a sheet

- Pull upward on part of a free edge – other 3 edges are fixed.



"Experimental data"



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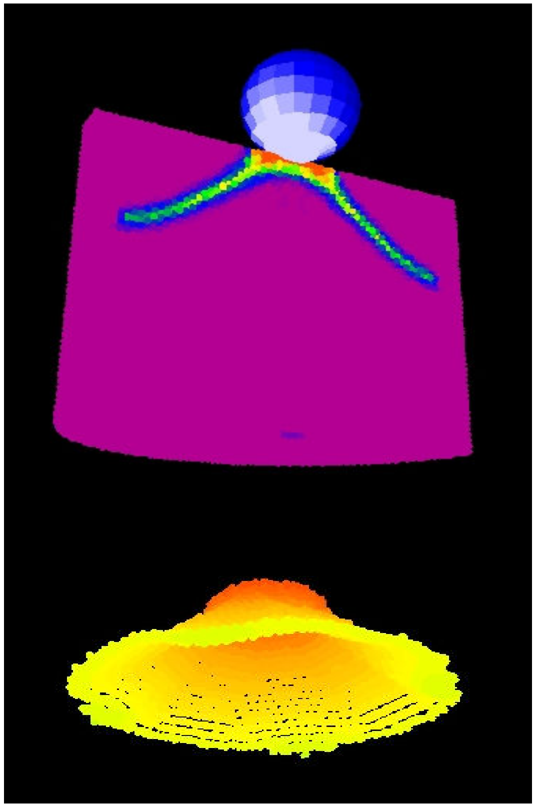
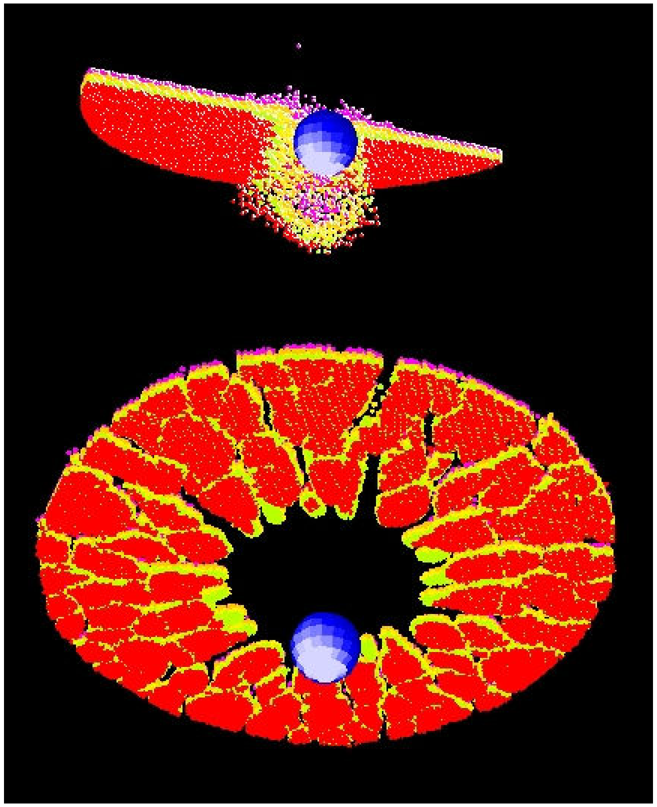
Hertzian cracking and fragmentation in glass



Low speed impact forms conical crack



Higher speed impact forms fragments

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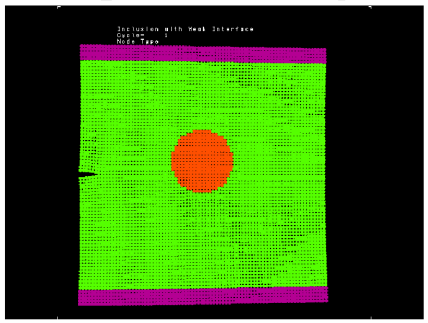
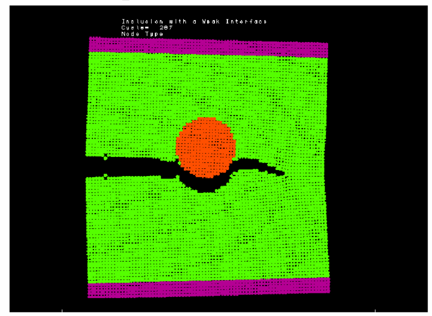
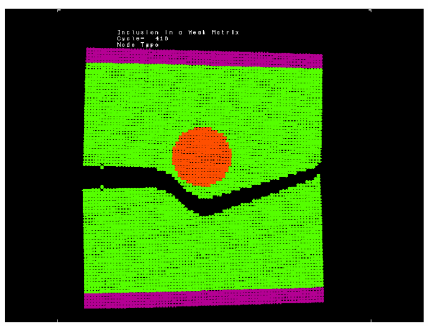
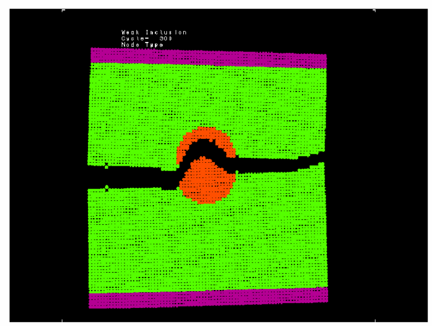
Treatment of interfaces

- Bonds connecting different materials can have properties independent of the constituent properties.
- Crack growth is “autonomous:” no need for supplemental kinetic relations.


Initial condition

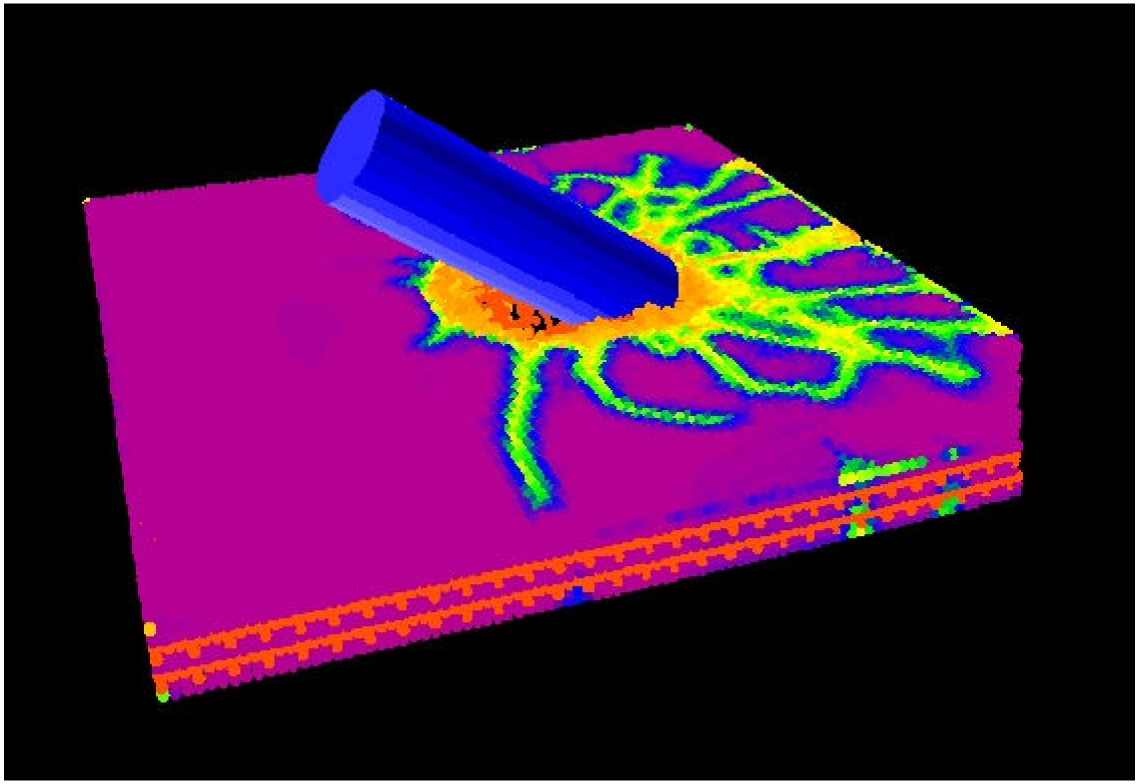

Weak interface


Weak matrix


Weak fiber

Impact onto reinforced concrete

- Reinforcement is modeled explicitly.



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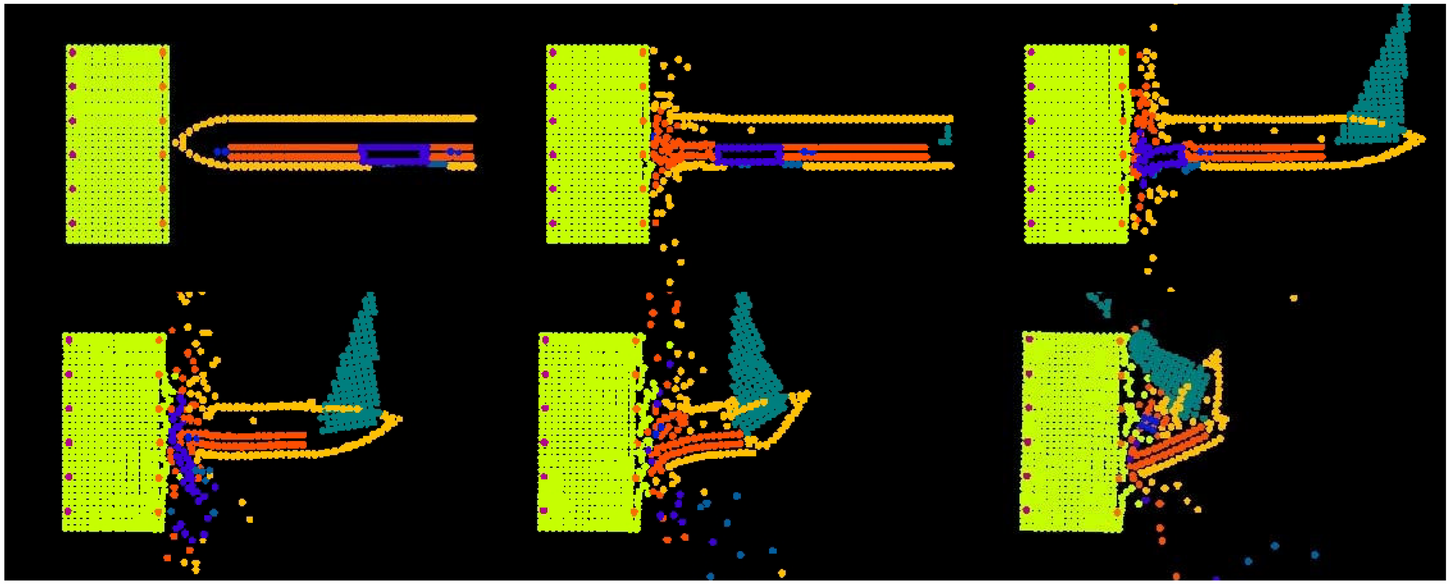
F4 airplane into concrete block



• EMU model of full-scale experiment (Sugano et al, Nuclear Engineering and Design 140 373-385 (1993).

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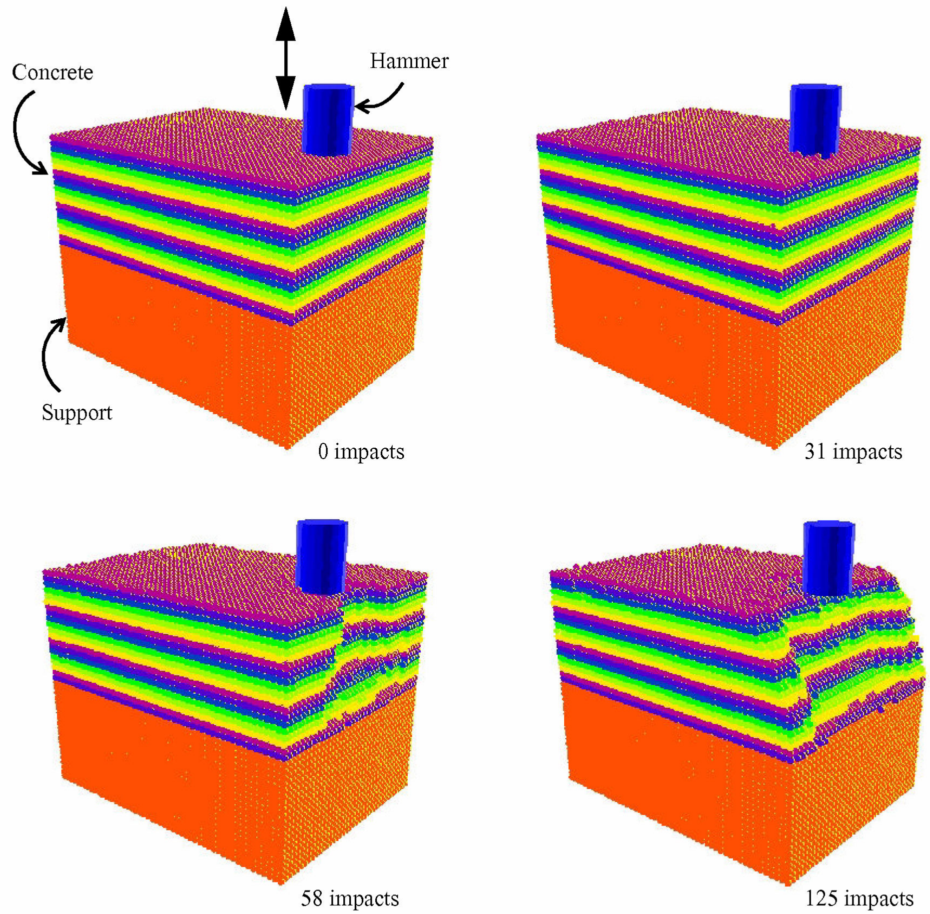
Damage accumulation due to repetitive impact (“jackhammer”)

• Each successive impact breaks more bonds internally.
• These coalesce into large cracks.



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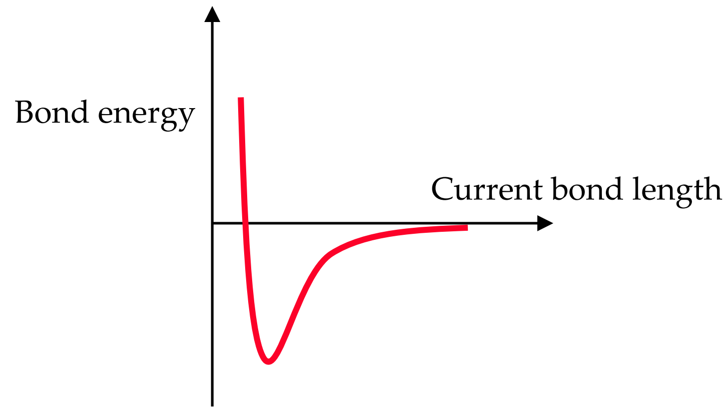
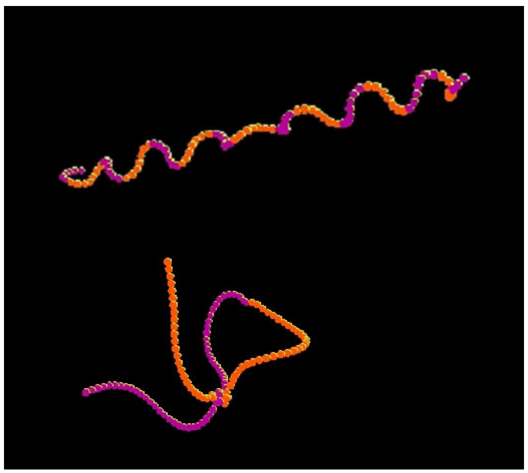
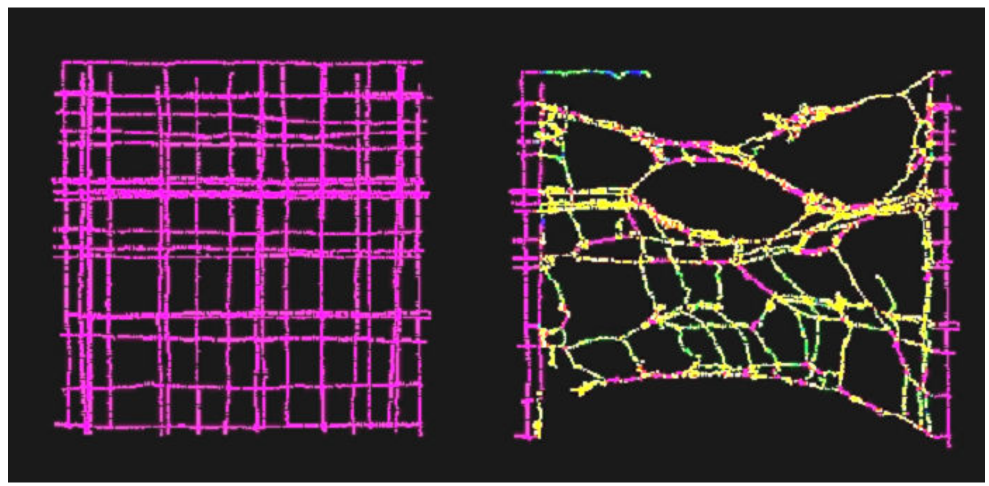
Fibers and fiber networks

- Long-range (e.g. van der Waals) forces treated the same way as peridynamic forces.





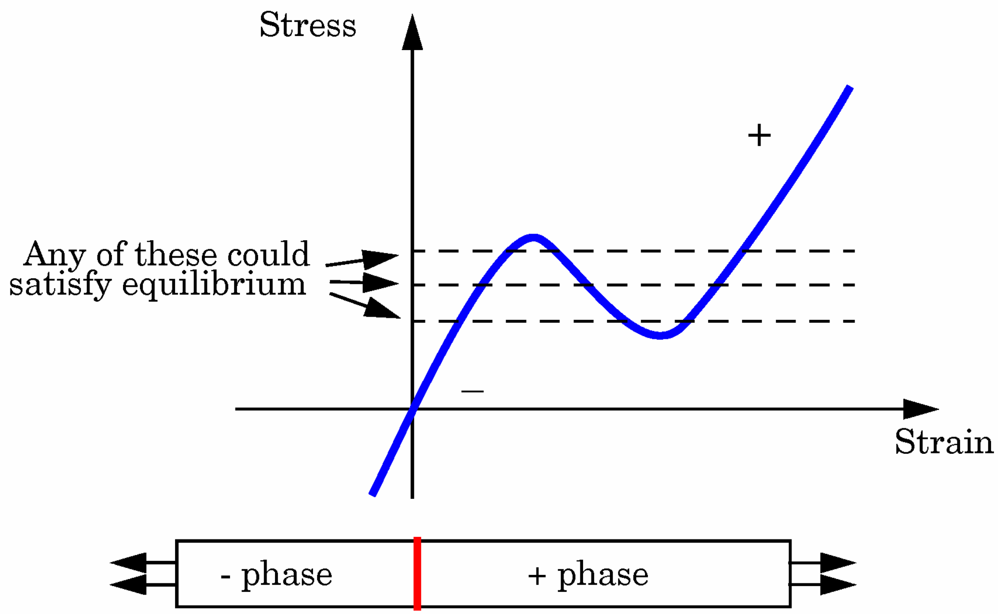
Fibers in which different segments attract or repel each other



Failure of a nanofiber network including VDW forces
(F. Bobaru, Univ. of Nebraska)

Phase boundaries: classical approach

- Classical theory:
  - Supplemental condition (such as the Maxwell condition) is required to determine the conditions at a phase boundary.



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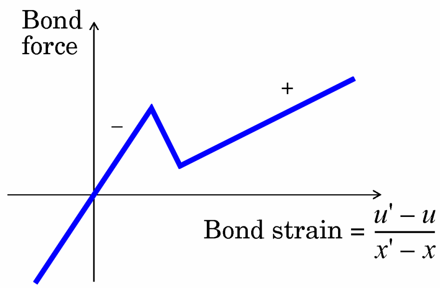
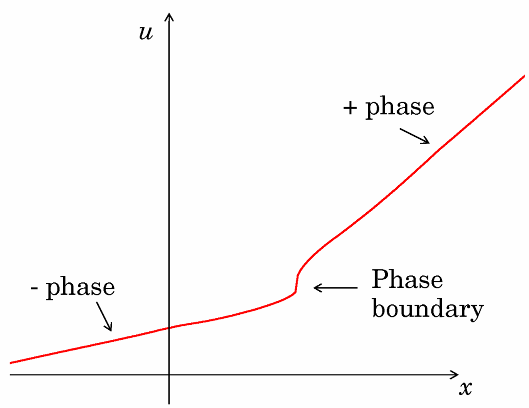
Phase boundaries: peridynamic

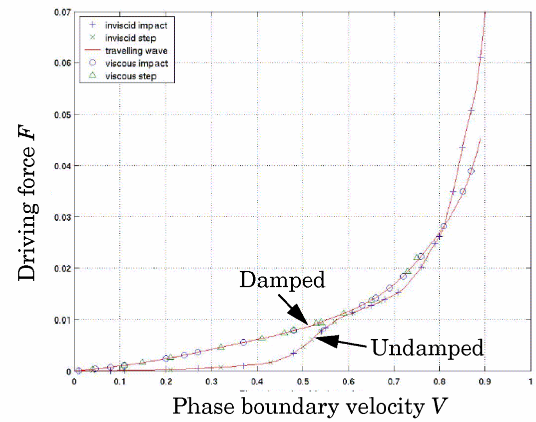
- Constitutive model:



- Numerical solution for static displacement field:



- Computed phase boundary velocity (for a specific material):



where the driving force (in the classical theory) is defined by
$$F = [W] - \langle\sigma\rangle[\varepsilon].$$

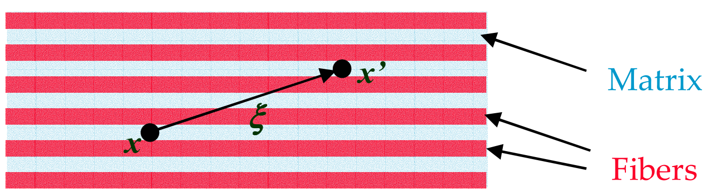
Peridynamic model appears to select particular conditions across the phase boundary (results of K. Dayal).

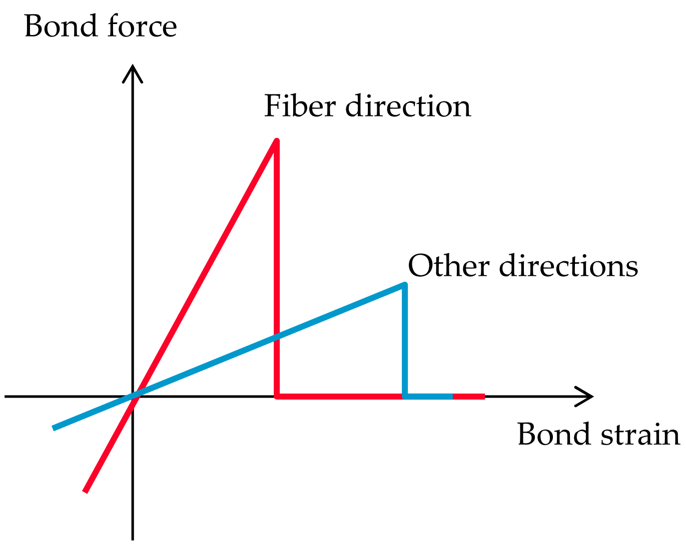
Laminated composite materials

- Recall that the bond force can depend on the separation <u>vector</u> ξ between $\boldsymbol{x}$ and $\boldsymbol{x}'$ in the reference configuration.

$$f(\eta, \xi)$$

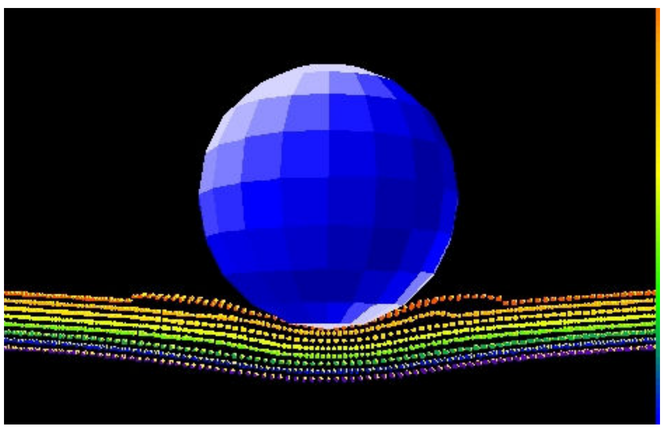
- Bonds in the fiber direction are stiffer and stronger than the others.
  - Micromodulus of each is fitted to bulk elastic modulus in each direction.
  - Interface bonds (connecting 2 different materials) can have properties independent of the others.



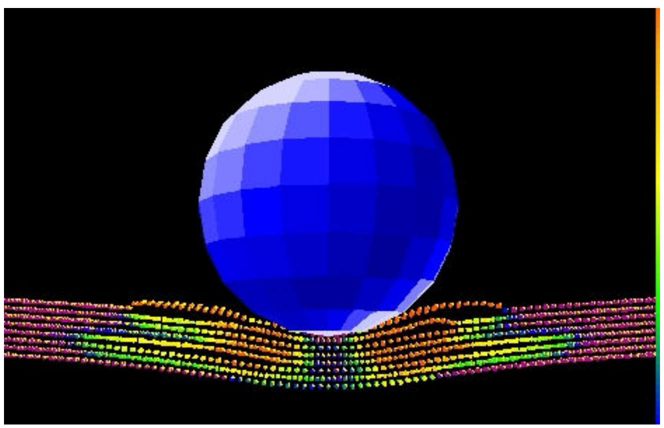


Impact on a laminated composite

- 25/50/25 stacking sequence, 32 layers, 1″ diameter projectile at 5.1 m/s).
- Note blistering near front surface due to delamination + buckling.
- Central area has less damage because of large out-of-plane compressive stress.
  - Also the shear stress vanishes along the central axis.



Colors indicate material (layer).

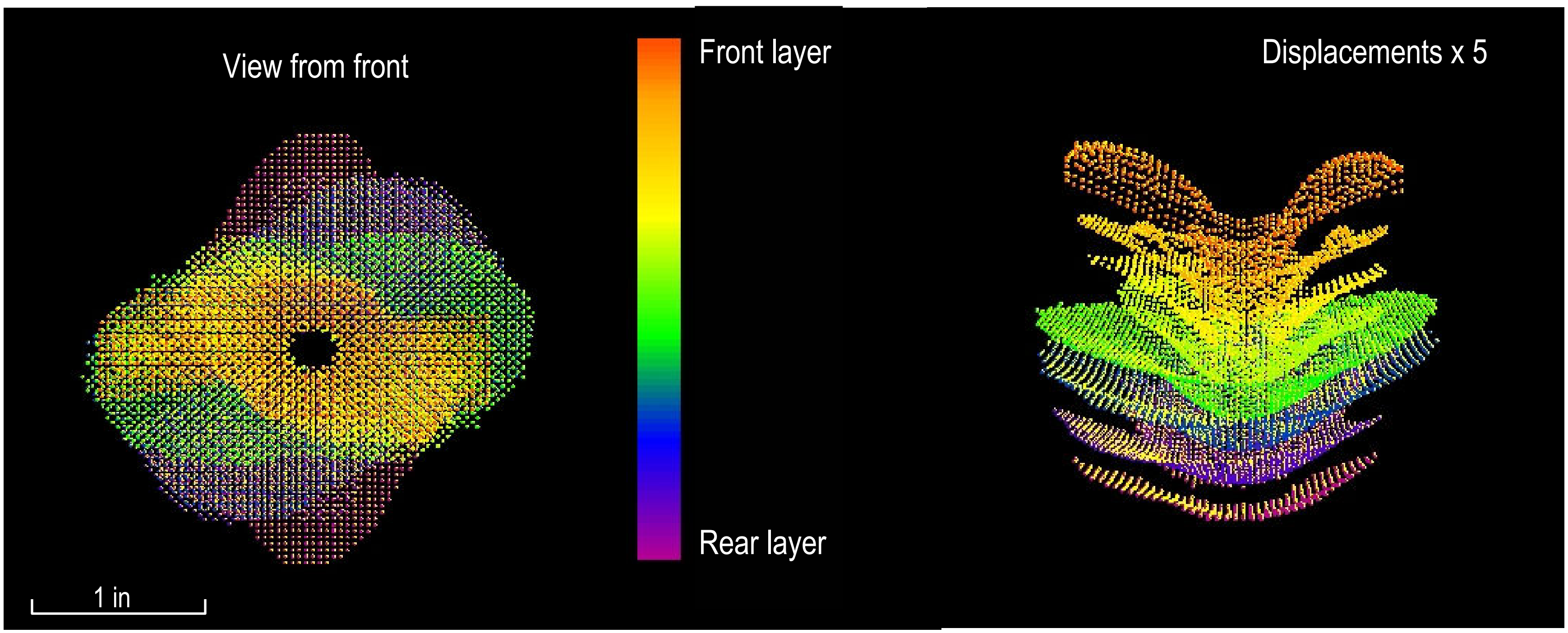


Colors indicate damage.

Both figures are at time of maximum penetration depth

Impact on a composite: Views of delaminated areas

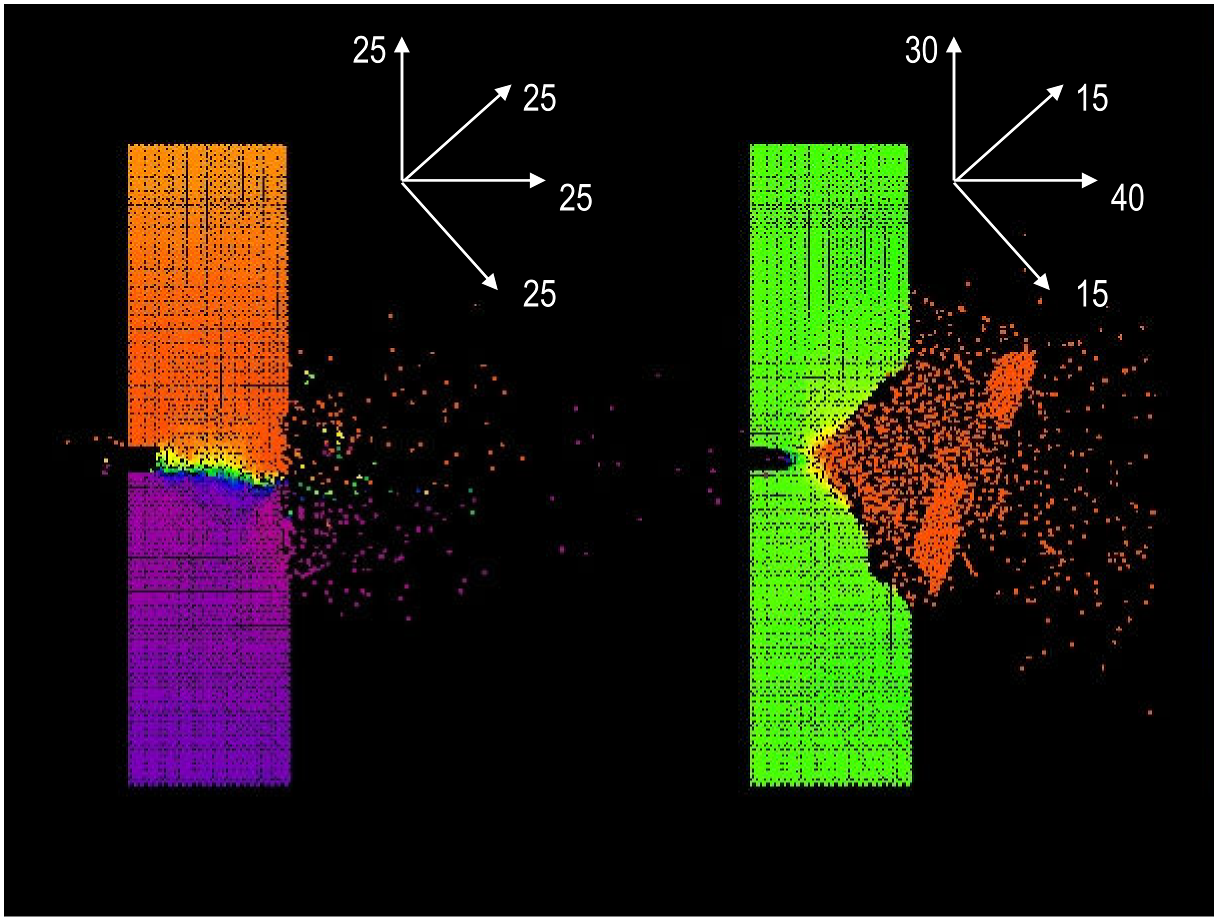
- Delaminations form in roughly elliptical regions.



Colors indicate material (layer)
Only damaged layers are shown.

Fracture modes in a laminated composite

- How does the makeup of a composite influence how it fails in a middle tension test (with a blunt notch)?



Some research issues

- Criteria for material stability and fracture:
  - Convexity of some quantity related to the micropotential?
- Plasticity with plastic incompressibility.
- Quantitative relationship with molecular dynamics.
  - Multiscale: method for “coarse graining”.
  - Nanoscale.
- Homogenization of heterogeneous materials.

For further information:

- www.sandia.gov/emu/emu.htm
- Email to sasilli@sandia.gov